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M. Hochlaf

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Potential energy functions and rovibrational spectra of the diaza−dicarbon (CCNN) and cyanogen (NCCN)

M. HOCHLAF

Theoretical Chemistry Group, Université de Marne−La−Vallée
F−77454 Champs−sur Marne, France.

The six dimensional PEFs of the ground state of CCNN and NCCN has been generated by the RCCSD(T) approach. The quartic force field in dimensionless normal coordinates has been evaluated. This force field has been used to calculate a set of spectroscopic constants. For NCCN, the quartic force field has been optimised using the experimental results and the full rovibrational spectrum is given with an accuracy better than 1 cm^{-1}. In the case of CCNN, the lowest singulet states are investigated. The ground state ($X^1\Sigma^+$) is found to be stable against dissociation into C_2 ($X^1\Sigma_g^+$) and N_2 ($X^1\Sigma_g^+$) and it presents a potential energy barrier due to an ovoided crossing with the excited $d^1\Sigma^+$ state. The other singulet states are found to be repulsive with respect to the dissociation into C_2 and N_2.